Eu's Generalized Hydrodynamics as the Basis of a New Computational Model for Rarefied and Microscale Gasdynamics

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Abstract. A new computational model based on Eu's generalized hydrodynamics, which has been recently proposed for describing the motion of gases in non-equilibrium state and is shown to be consistent with the second law of thermodynamics, is presented. The general understanding of Eu's generalized hydrodynamics, which employs the cumulant expansion for the Boltzmann collision integral instead of the BGK approximation, is also obtained by considering three fundamental flows; compressed gas in shock waves, expanding gas, and velocity shear flow. The study on these problems reveals that Grad's equations are similar to Eu's equations in the slip flow, but become drastically different from Eu's equations in shock structure problem. A plausible explanation is that the relaxation time approximation may be insufficient in modeling the extreme nonlinearity of shock structure since the Boltzmann collision integral plays a critical role in this case. Finally, by considering the microscale channel flow, a new slip boundary condition based on Langmuir's theory is presented that predicts a trend of increasing pressure curve nonlinearity with increasing rarefaction and a minimum in mass flow rate, which are not the case with the results predicted by the first-order Maxwell slip condition.

INTRODUCTION

Analysis of high thermal non-equilibrium gas flows in many instances requires mathematical models beyond the Navier-Stokes equations. Many computational models–either fully kinetic (DSMC) or fluid dynamic (moment equations)–have been proposed, but it turned out that some have difficulty in solving low-speed micro-scale flow and others suffer non-trivial problems: violation of the 2nd law of thermodynamics, closure breakdown, and trouble in boundary condition. This status is somewhat surprising since the fluid dynamic approach is simply to solve the following collision-free hyperbolic conservation laws,

$$\frac{\partial}{\partial t}\int_V \mathbf{U}dV + \oint_S \mathbf{F}\cdot\mathbf{n}dS = 0, \tag{1}$$

where S represents the bounding surface of the control volume V, and $\mathbf{U}$ represent conserved variables $(\rho, \rho\mathbf{u}, \rho E)$. $\mathbf{F}$ in the surface integral represents the flux consisting of non-conserved variables (stress and heat flux) and conserved variables. Here it should be emphasized that these laws are the exact consequence of both kinetic theory and continuum mechanics. Only after some approximations are made to non-conserved variables, they become approximate fluid dynamic equations, for example, the Navier-Stokes equations. It was found, however, that the procedure to calculate non-conserved variables is not simple, and indeed it is generally believed that there exist no high-order equations fully consistent with the macroscopic and phenomenological thermodynamics.

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14. ABSTRACT
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EU'S GENERALIZED HYDRODYNAMICS

Towards solving this dilemma, an alternative and yet unknown method in which the second law of thermodynamics is satisfied to every order of approximation, the Eu's generalized hydrodynamics (GH) [1] is considered in this study as the basis of a new computational model for high non-equilibrium gas flows. The essence of his theory can be summarized as follows. Starting from the following irreversible thermodynamics

$$Td\Psi = dE + pdV + \sum X^{(\alpha)} \odot d < \Phi^{(\alpha)}/\rho >, \tag{2}$$

which is equivalent to an exponential form of the distribution function

$$f = f^{(0)} e^{-[\sum X^{(\alpha)} \odot h^{(\alpha)} - \mu]/k_B T}, \tag{3}$$

a thermodynamically consistent hydrodynamic equations can be developed. Ψ in the equation (2) represents a non-equilibrium entropy that recovers the equilibrium entropy S for an equilibrium system. $\Phi^{(\alpha)}$ represent high-order moments such as stress and heat flux, while $X^{(\alpha)}$ represent tensors whose role is similar in the coefficients of conventional expansion methods. A leading term $X^{(1)}$ can be written as $-\mathbf{\Pi}/(2p)$, where $\mathbf{\Pi}$ represents stress tensor. $h^{(\alpha)}$ is directly related to $\Phi^{(\alpha)}$ through the relation $\Phi^{(\alpha)} =< h^{(\alpha)} f >$. μ is the normalization factor. The essence of the Eu's generalized hydrodynamics can be found in an exponential form of the distribution function (3). The use of the exponential form makes it possible to apply the cumulant expansion and ensures that the approximated distribution functions always remain non-negative. Note that f can never be negative and must either have finite bounds in velocity space or tend to zero as a particle velocity tends to infinity. This point can be highlighted by realizing that the following conventional polynomial expansions show the poor convergence, meaning that there always exists a region in which the function can be either negative or unbounded.

$$f = f^{(0)} + \mathrm{Kn} f^{(1)} + \mathrm{Kn}^2 f^{(2)} + \cdots. \tag{4}$$

Thus, it is the exponential form of the distribution function that distinguishes the Eu's GH from the rest of other hydrodynamic approaches.

One of the simple form of GH constitutive relations retaining the essence of theory can be written as [2,3]

$$\hat{\mathbf{\Pi}}\, q(c\hat{R}) = \hat{\mathbf{\Pi}}_{\mathrm{NS}} + [\hat{\mathbf{\Pi}} \cdot \nabla \hat{\mathbf{u}}]^{(2)}, \tag{5}$$

$$\hat{\mathbf{Q}}\, q(c\hat{R}) = \hat{\mathbf{Q}}_{\mathrm{NS}} + \hat{\mathbf{\Pi}} \cdot \hat{\mathbf{Q}}_{\mathrm{NS}}, \tag{6}$$

where $\mathbf{\Pi}_{\mathrm{NS}} = -2\eta[\nabla \mathbf{u}]^{(2)}$, $\mathbf{Q}_{\mathrm{NS}} = -\lambda \nabla \ln T$, $\hat{\mathbf{\Pi}} \equiv \frac{N_\delta}{p}\mathbf{\Pi}$, $\hat{\mathbf{Q}} \equiv \frac{N_\delta}{p}\frac{\mathbf{Q}}{\sqrt{T/(2\epsilon)}}$, $\nabla \hat{\mathbf{u}} = -2\eta \frac{N_\delta}{p} \nabla \mathbf{u}$, $\hat{R}^2 = \hat{\mathbf{\Pi}} : \hat{\mathbf{\Pi}} + \hat{\mathbf{Q}} \cdot \hat{\mathbf{Q}}$, $q(c\hat{R}) = \frac{\sinh(c\hat{R})}{c\hat{R}}$. Here $\mathbf{Q}$ represents heat flux vector.

A constant c has a value between 1.014 (Maxwellian) and 1.223 (ν=3), where ν is the exponent of the inverse power laws of gas particles and $s = 1/2 + 2/(\nu - 1)$. In case of helium gas, c becomes 1.046($\nu = 14$). η and λ are the Chapman-Enskog viscosity and thermal conductivity . They can be expressed as $\eta = T^s$, $\lambda = T^{s+1}$. For a monatomic gas, $\gamma = 5/3$ and $\mathrm{Pr} = 2/3$. A composite number, which is defined as $N_\delta \equiv \eta u/(pL) \sim \mathrm{Kn}M$ and appears in the term $X^{(1)}$, measures the magnitude of the viscous stress relative to the hydrostatic pressure, so that it indicates the level of departure from thermal equilibrium. When the new constitutive relations (5) and (6) are compared with Grad [5] and Burnett [7] equations, several interesting results can be found. In multi-dimensional flows, the following three cases can be considered most basic flows.

Shock Wave and Gaseous Expansion When the gas experiences compression or expansion, the gradient of normal velocity will remain either negative or positive. In these cases ($\partial u/\partial x$ only), the Eu's, Grad's, and Burnett's relations for the normal stress reduce to

$$\hat{\Pi}_{xx} q(c\sqrt{\frac{3}{2}}\hat{\Pi}_{xx}) = (1 + \hat{\Pi}_{xx})\hat{\Pi}_{xx_{\mathrm{NS}}}, \quad \hat{\Pi}_{xx} = \frac{4\hat{\Pi}_{xx_{\mathrm{NS}}}}{4 - 7\hat{\Pi}_{xx_{\mathrm{NS}}}}, \quad \hat{\Pi}_{xx} = (1 + \hat{\Pi}_{xx_{\mathrm{NS}}})\hat{\Pi}_{xx_{\mathrm{NS}}}. \tag{7}$$

In Fig. 1 (a), Eu's and Grad's results for the normal stress are plotted. It can be observed that Eu's relation is well-defined in all non-equilibrium states. Note that the Grad's equation has a non-removable singularity at $\hat{\Pi} = 4/7$ in positive region (shock wave) and the Burnett's equation loses one-to-one correspondence in

negative region (expanding gas), which in turn implies the violation of positive entropy production [7]. Even though the algebra in these relations is quite simple, it turns out that the results are very general. In the previous work [4], it was found that even if heat flux is included, the general characteristics remain unchanged. Furthermore, an independent calculation done by Karlin *et al.* [8] confirms this characteristics. They extended the hydrodynamic description into a highly non-equilibrium domain by summing all the relevant subseries of the original Chapmann-Enskog expansion from the Grad equations and obtained the following linear relation for Maxwellian molecules,

$$\hat{\Pi}_{xx} = \frac{1}{2\hat{\Pi}_{xx_{\rm NS}}}\left[\hat{\Pi}_{xx_{\rm NS}} - 2 + [(\hat{\Pi}_{xx_{\rm NS}} - 2)^2 + 8\hat{\Pi}^2_{xx_{\rm NS}}]^{1/2}\right]. \tag{8}$$

It can be easily shown that this relation is very similar to the GH relation, even though some details are different.

The salient feature of the GH equation is that it recovers the free-molecular limit in gaseous expansion and shows high nonlinearity in gaseous compression. It can be induced from this nonlinearity that there must exist at least one region of shock wave structure in which the actual stress is greater than the stress calculated by the Navier-Stokes equations, irrespective of Mach numbers. It is exactly this nonlinearity that makes the GH solutions for shock structure in strong agreement with experimental data [6,2]. Notice that the essential contribution to this nonlinearity comes from terms $q(c\hat{R})$ and $[\hat{\mathbf{\Pi}} \cdot \nabla \hat{\mathbf{u}}]^{(2)}$, which represent energy dissipation by particle collision and the strong coupling between the stress and velocity gradient. On the other hand, the work by Karlin *et al.* implies that summation of all the relevant terms is necessary to explain the extreme nonlinearity of shock structure. This point may explain a consistent finding that the common relaxation time (BGK) approximation for the Boltzmann collision integral yields poor results in high Mach shock structure problem.

Velocity Shear Flow When there exists the gradient of shear velocity only ($\frac{\partial v}{\partial x}$ only), the Eu's, Grad's and Burnett's relations reduce to

$$\hat{\Pi}_{xx} = -\frac{2\hat{\Pi}^2_{xy_{\rm NS}}/3}{q^2(c\hat{R}) + 2\hat{\Pi}^2_{xy_{\rm NS}}/3}, \quad \hat{\Pi}_{xx} = -\frac{2\hat{\Pi}^2_{xy_{\rm NS}}/3}{1 + 2\hat{\Pi}^2_{xy_{\rm NS}}/3}, \quad \hat{\Pi}_{xx} = -0.733\hat{\Pi}^2_{xy_{\rm NS}}, \tag{9}$$

where $\hat{R}^2 = 3\hat{\Pi}_{xx}(\hat{\Pi}_{xx} - 1)$ and with the same stress eclipse in Eu's and Grad's cases,

$$\hat{\Pi}_{xy} = \text{sign}(\hat{\Pi}_{xy_{\rm NS}})[-\frac{3}{2}(1 + \hat{\Pi}_{xx})\hat{\Pi}_{xx}]^{1/2}.$$

It can be shown in Fig. 1 (b) that the behavior of stresses becomes very different from the Navier-Stokes description in highly non-equilibrium states. The normal stress is generated by the shear velocity gradient and the shear stress approaches zero as the velocity gradient increases. This asymptotic behavior means that the gas slips near the solid wall. As a result, the velocity-slip phenomenon can be explained in purely hydrodynamical terms. Notice also that Eu's results are very similar to Grad's results, except for the existence of a nonlinear term $q(c\hat{R})$ that comes directly from the Boltzmann collision integral. This similarity, which is not the case in shock structure problem, can be explained by the existence of the stress eclipse. It must be noticed that the kinematic relations are solely responsible for this stress constraint, not the collision integral terms. Therefore it is not surprising to find out that the BGK approximation yields fairly good results in the boundary layer flow, which is dominated by the velocity shear flow.

Multidimensional Flow Even though the new equations can explain nonlinear transport of gas in non-equilibrium state, a proper computational method must be developed in order that they may serve as a tool for the simulation of gas flows in multidimensional geometry. In the previous work [3], an idea to overcome the difficulty of multidimensional extension caused primarily by the existence of highly nonlinear terms has been proposed. On the basis of such idea, a numerical solution of the equations (1), (5), and (6) was obtained for the two-dimensional flow over a flat plate with $M = 12.9$ and $\text{Kn} = 0.0067$. The important finding was that the GH calculation produces results very close to physical intuition, removing the singularity near the leading edge that is ill-defined in continuum gas dynamics. The ultimate reason for this can be traced to the fact that the shear stress measured by the GH equations, shown in Fig. 1 (b), are nonlinearly related to the gradient of velocity, smaller than that measured by the NS equations in high non-equilibrium flow regions.

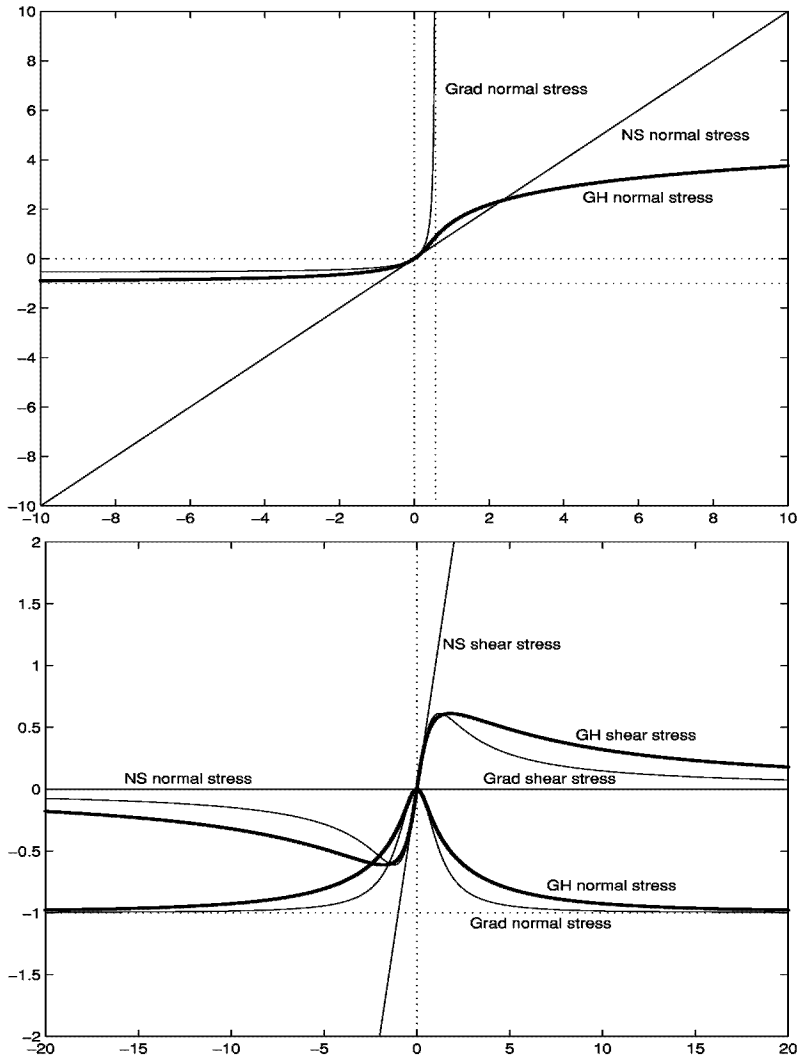

FIGURE 1. (a) Eu's GH relation relative to the Navier-Stokes relation in the region of compressed (positive) and expanding (negative) gas (no heat flux for simplicity). The horizontal axis represents the velocity gradient (top). (b) The normal and shear stresses described by Eu's GH and Grad's equations (bottom).

MEASURE OF THERMAL NON-EQUILIBRIUM

According to the conventional non-equilibrium theory based on the mean free path, gas flows encountered in low-density environments and microscale geometries at standard atmospheric conditions can be treated with no difference and requires the mathematical models beyond the continuum description. Therefore, it is natural to argue that DSMC or high-order moments equations should be used to simulate microscale gas flows with high Knudsen numbers. There exists, however, an ambiguity in using the mean free path as the parameter to classify non-equilibrium gas flow regimes. For example, there are many calculations in which the problem with a smaller Knudsen number shows high non-equilibrium effects than the problem with a higher Knudsen number. In fact, the classification based on the Knudsen number is largely empirical and depends highly on the problem considered. This is not surprising at all if we recall the physical reasoning that the gas flows associated with microscale geometry at normal pressure, which is typical in most of MEMS devices, is perfectly near equilibrium unless the gas-surface interaction has long-range effects on the overall flow structure. It is well known, however, that the scale length associated with the gas-surface interaction (due to physical force) is order of molecular size (nanoscale).

This reasoning may give a hint of a possibility of developing a better measure of thermal non-equilibrium

in gas flows. Indeed, if the GH equations (5) and (6) are carefully examined, it becomes immediately evident that a composite number N_δ, which is defined as

$$N_\delta \equiv \frac{\eta_r u_r}{p_r L} = \frac{\gamma M^2}{\mathrm{Re}} = \mathrm{Kn} M \sqrt{\frac{2\gamma}{\pi}},$$

indicates the level of departure from thermal equilibrium. When N_δ is small, the GH constitute relations recover the Navier-Stokes relations. This can also be confirmed from the graphical representation of the GH relations (Fig. 1).

Even though this finding appears trivial, it has huge implications. The most obvious one is that the classification of bulk flow regimes should be based on the Knudsen number times the Mach number, not Knudsen number alone. In order to explain this, let us consider a typical rarefied flow, for example, a hypersonic flow over a vehicle flying at an altitude of 93 km. For realistic values of flight conditions (length = $1m$, velocity= $8km/s$), dimensionless parameters can be approximated as

$$\mathrm{Kn} = 0.037,\ N_\delta = 1.0.$$

On the other hand, for helium gas flow in a typical microchannel (length = $1.2\mu m$, exit velocity = $50cm/s$), they are

$$\mathrm{Kn} = 0.145,\ N_\delta = 7.67 \times 10^{-5}.$$

According to the new picture, there is no need of using the high-order equations in microscale gas flows since N_δ is extremely small. Notice that N_δ will remain relatively small for low-speed flow even when the channel height is measured on a nanoscale. The Navier-Stokes relations will be just enough to calculate these flows if the slip effect on the solid surface due to high Knudsen number is properly taken into account. However, this line of thinking has not been validated, primarily due to the lack of proper slip boundary conditions.

MICROSCALE GAS FLOWS

The lack of proper slip boundary condition can be manifested when a benchmark problem is considered, namely, internal gas flows in microchannels. For the sake of simplicity, let us consider a long microchannel with the ratio of the channel height (H) to its length (L) ε in isothermal condition ($273K$). Using the method described by Arkilic *et al.* [11], the Navier-Stokes equations, at the zeroth order, may be written as

$$\varepsilon \frac{\partial (pu)}{\partial x} + \frac{\partial (pv)}{\partial y} = 0, \tag{10}$$

$$\frac{\varepsilon}{N_\delta} \frac{dp}{dx} = \frac{\partial^2 u}{\partial y^2}. \tag{11}$$

The streamwise coordinate x and the wall-normal coordinate y are nondimensionalized by L and H, respectively. The reference state is chosen as the outlet conditions. The reference velocity is the area-average streamwise velocity at the channel exit. The solutions to these equations can be obtained by either numerical methods or analytical methods if boundary conditions on the solid wall are specified.

Maxwell Slip Boundary Conditions The Maxwell slip boundary condition has been popular in the past owing to its simplicity. It is largely based on the notion of accommodation coefficients which measure the fraction of molecules undergoing diffusive reflection. It turned out in the present problem that the first-order Maxwell slip condition,

$$u_{\mathrm{boundary}} = \sigma \frac{\mathrm{Kn}}{p} \frac{\partial u}{\partial y}\bigg|_{\mathrm{boundary}}, \tag{12}$$

yields simple analytic solutions of velocity profile and mass flow rate,

$$u(x,y) = -\frac{3}{\delta}\frac{dp}{dx}\left[1 - 4y^2 + 4\sigma\frac{\mathrm{Kn}}{p}\right],\ \dot{m} = \frac{1}{\delta}(p_{\mathrm{in}} - 1)(p_{\mathrm{in}} + 1 + 12\sigma\mathrm{Kn}). \tag{13}$$

Here $\delta = 24N_\delta/\varepsilon$, $p_{x=0} = p_{\text{in}}$, $p_{x=1} = 1$, and σ represents the streamwise momentum accommodation and is often taken as $\sigma = 1$. It was found from these solutions that the prediction by the first-order Maxwell condition is in strong agreement with experimental observations, in particular, the streamwise velocity profile and the nonlinear pressure distribution along the channel. However, it was also found that this condition cannot predict the existence of a minimum in mass flow rate in the transition region, which highlights the essential nonlinearity of slip phenomenon. In addition, a careful examination revealed qualitatively different results with experimental findings and physical intuitions. For example, it predicted a pressure distribution with smaller nonlinearity in more rarefied flows, suggesting that rarefaction negates compressibility, in contradiction to experimental results and physical intuition. It also predicted a drift of mass toward the wall as the flow progresses down the channel, in contrast with the physical picture which can be induced from approximating the channel flow by Blasius profiles along two flat plates.

In order to overcome these limitations, the high-order Maxwell conditions have been proposed by Beskok *et al.* [13]. It was shown that the high-order conditions predict the existence of a minimum in mass flow rate. It is not clear, however, that they can predict the free-molecular limit of mass flow rate and solve the problems described in previous paragraph.

Langmuir Slip Boundary Condition Even though the description of slip phenomenon by Maxwell is simple, there exist non-trivial issues. For example, it lacks the predictability since this condition requires some adjustable parameters in the form of accommodation coefficients, which is highly dependent of type of gases and wall materials and geometry. It can also be noticed that the slip velocity by this condition is unbounded, which may cause unphysical high slip velocity and affect the type of vorticity near the wall. Finally, it is susceptible to the numerical errors by under-resolved calculation of the derivatives of tangential velocity near the wall. Here a simple slip boundary condition based on the theory of adsorption phenomena developed by Langmuir [9,10] will be considered. This condition has been implemented in the simulation of rarefied hypersonic flow over a flat plate [3] and microscale gas flows [4].

This condition is based on the theory of adsorption phenomena pioneered by Langmuir. In his historic work of molecular films of gases on solid surfaces, he developed a conception of adsorption phenomena. According to his description, gas molecules do not in general rebound elastically, but condense on the surface, being held by the field of force of the surface atoms. These molecules may subsequently evaporate from the surface, resulting in some time lag. Adsorption and slip is the direct result of this time lag. From this physical reasoning, he derived the following equation of the fraction of surface covered at equilibrium, which is of far-reaching significance in surface chemistry,

$$\alpha = \frac{\beta p}{1 + \beta p}. \tag{14}$$

Here an expression of β,

$$\beta = \frac{A l_r}{k_B T_w} e^{\frac{D_e}{k_B T_w}} \frac{\ell}{l_r},$$

can be introduced. A is the mean area of a site, D_e is the potential parameter and they can be inferred from either theoretical prediction or experimental data. l is the mean free path, and k_B is the Boltzmann constant. ℓ is a mean collision distance between the wall surface and the gas molecules at all angles. With α calculated, the boundary values of dimensionless velocity can be determined by

$$u = (1 - \alpha) \text{ or } u_{\text{boundary}} = \frac{1}{1 + \beta p} \text{ in the present case,} \tag{15}$$

where $\beta = 1.28/\text{Kn}$ for He-Al.

It can be easily shown that this new condition yields the following results [4],

$$u(x,y) = -\frac{3}{\delta}\frac{dp}{dx}(1 - 4y^2) + \frac{1}{1 + \beta p}, \; \dot{m} = -\frac{2}{\delta}\frac{dp}{dx}\Big|_{x=1} + \frac{1}{1+\beta} = \frac{1}{\beta} + s, \tag{16}$$

where a quantity s defined as $\left[-2\frac{dp}{dx}\Big|_{x=1} - \frac{\delta}{\beta(\beta+1)}\right]$ satisfies a nonlinear equation

$$\beta^3 \delta s^2 - \beta^3 (p_{\text{in}}^2 - 1)s + 2\beta(p_{\text{in}} - 1) - 2(1 + \frac{1}{\beta s})\ln\frac{\beta(\beta p_{\text{in}} + 1)s + 1}{\beta(\beta+1)s + 1} = 0.$$

Surprisingly, it can be shown that these solutions explain all the contradictory problems. The new theory predicts that the nonlinearity in pressure distribution increases as the Knudsen number increases. In addition, the new theory shows that there always exists a drift of mass from the wall and its magnitude is much smaller than one predicted by the Maxwell slip condition. Lastly, it can be easily shown in the relation (16) that there always exists a minimum in mass flow rate in transition regime. This critical property can be seen in Fig. 2 where the flow rate exhibits a correct continuum limit and an algebraic singularity at very high Knudsen number,

$$\dot{m}_{\text{continuum}} \to \frac{p_{\text{in}}^2 - 1}{\delta}, \quad \dot{m}_{\text{free-molecular}} \to \frac{p_{\text{in}}}{1 + \beta p_{\text{in}}}. \tag{17}$$

In fact, the mass flow rate can be expressed as three parts; continuum and slip (slip + self-diffusion).

$$\dot{m} = \dot{m}_{\text{continuum}} + \dot{m}_{\text{slip}} + \dot{m}_{\text{self-diffusion}}, \tag{18}$$

where

$$\dot{m}_{\text{slip}} = -\frac{2}{\delta}\left[\frac{p_{\text{in}}^2 - 1}{2} + \frac{dp}{dx}\bigg|_{x=1}\right], \quad \dot{m}_{\text{self-diffusion}} = \frac{1}{1+\beta}.$$

Note that $\dot{m}_{\text{self-diffusion}}$ is independent of the pressure difference and remains finite in non-continuum regime even for constant pressure. This conclusion agrees well with the explanation advanced by Liu [12].

SUMMARY

A new computational model fully consistent with the second law of thermodynamics is presented. Through a critical review of the previous models on basic flows, the characteristics of the new model are identified. The important finding is that the level of thermal non-equilibrium can be measured by the composite number N_δ and consequently the Navier-Stokes equations with proper slip boundary conditions can describe most of microscale gas flows. This point is demonstrated by developing the new slip boundary condition based on the Langmuir theory of the adsorption of gases on metals as monatomic films. It is shown that all the critical features including the existence of the minimum in mass flow rate can be explained by this simple condition.

It is also worthwhile mentioning that the approach taken in the present study holds for diatomic gases and dense gases and therefore the essence of the present work can go over to these gases. The results to these problems will be reported in due course.

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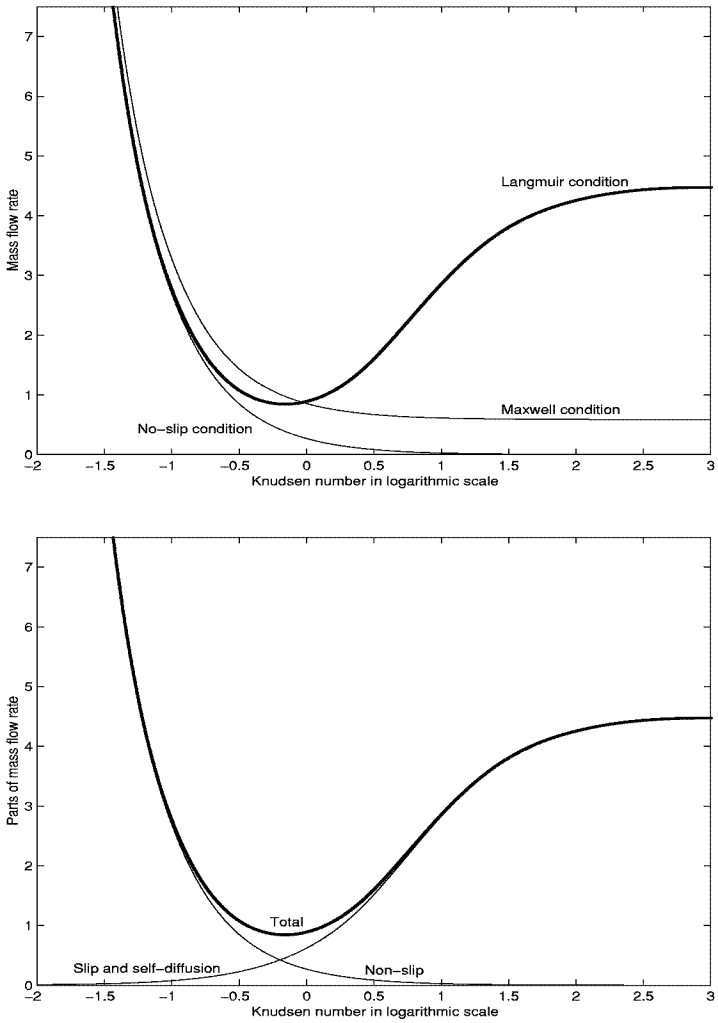

FIGURE 2. (a) Variation of mass flow rate as a function of exit Knudsen number in the microchannel (top). (b) Variation of components (continuum and slip) of mass flow rate in Langmuir's boundary condition (bottom).

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